Presence of Zero-Energy Cap-States in Carbon Nanotubes

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A closed structure at the end of a carbon nanotube is called a "cap." Such a cap usually contains six five-membered rings [1] and various cap structures can be made by different configurations of these five-membered rings. Peculiar states are present in caps such as localized states [2,3] and resonance states [4]. The purpose of this work is to study the dependence of such cap states on the cap structure.

In previous works, localized cap states were studied for caps consisting of q regular triangles in a tight-binding (TB) and an effective-mass approximation (EMA). This type of a cap, called the q-regular cap, has q five-membered rings at the boundary with a tube and a q-membered ring at the tip. In this paper, we study cap states for caps having more than two five-membered rings near their tip instead of q-membered rings. An example of the development such caps (called *star cap*) is shown in Fig. 1(a). Apart from the presence of three five-membered rings near the tip, this *star cap* is topologically equivalent to a 3-regular cap.

Figure 1(b) compares the results between caps consisting only of five-membered rings and corresponding q-regular caps, where results of q-regular caps correspond to discrete values of a continuous angular momentum σ_ϕ in the presence of a flux passing through the tip region in the 6-regular cap. It shows that the energy level of the star cap $\{3;3\}_3^{3v}$, for example, lies near the energy $\varepsilon = 0$ in disagreement with those for the 3-regular cap which lie near the valence and conduction band edges. Similar disagreement is present for other types of caps with $q = 2$ and 4.

In q-regular caps, the singularity of the wave function is restricted by various conditions including the normalizability. As shown in Fig. 1(b), cap states near zero energy disappear when σ_ϕ exceeds a certain critical value close to 3/2, where the singularity of the zero-energy wave function becomes too strong at the tip [3]. The presence of several five-membered rings in the vicinity of the tip effectively removes the tip region with the singular amplitude and therefore make cap states reappear at zero energy.

Figure 2 shows an average amplitude of the localized states for the star cap $\{3;3\}_3^{3v}$. It is defined by the average of the amplitude over all x lattice points on the line at given y where x and y is in the circumference and the axis directions, respectively, as shown in Fig. 1(a). It shows that the amplitude behaves as $|y|^{-1}$. Such a singular function should be excluded in a 3-regular cap containing the singular point $y = 0$ because it violates the normalizability, but becomes allowed in the star cap which does not contain $y = 0$.

References

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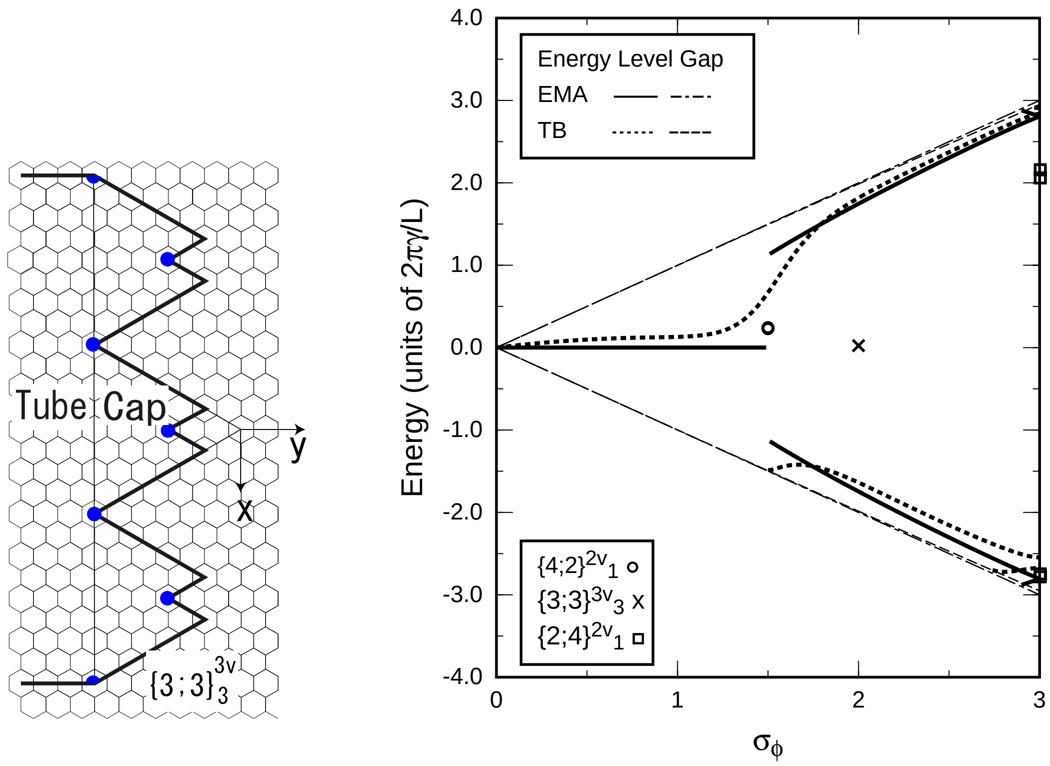

(a) (b)

Fig. 1 (a) A star cap $\{3;3\}_3^{3v}$. (b) Comparisons of the energy levels of some caps such as the star cap $\{3;3\}_3^{3v}$ ($\times$) with those of a 6-regular cap in presence of the magnetic flux passing through the cap tip (solid lines in TB and the dotted lines in EMA).

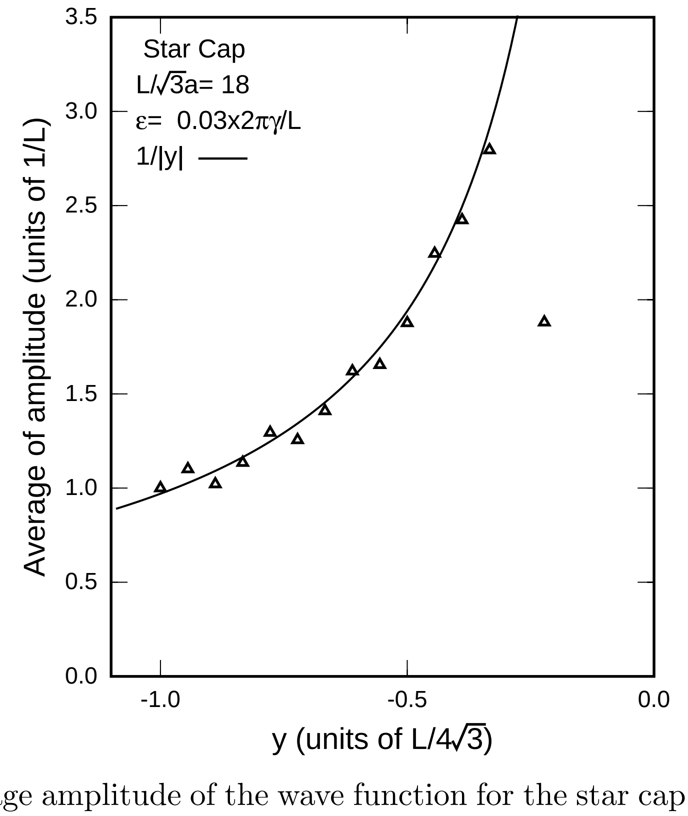

Fig. 2 An average amplitude of the wave function for the star cap $\{3;3\}_3^{3v}$ is shown by triangles at each y. y is defined in Fig. 1 (a). The solid line shows $c/|y|$ with c being an appropriate constant.